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Theoretical Analysis of the Rotational Barrier in Ethane: Cause and Consequences

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Supplementary Material

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Table S1. Optimized C–C and C–H bond lengths, d_{CC} and d_{CH} (Å), CCH and HCH bond angles, τ_{CCH} and τ_{HCH} (°), for staggered (S) and eclipsed (E) conformations of ethane and differences between E and S (Δ_{E-S}).

Conformation	Method	d_{CC}	d_{CH}	τ_{CCH}	τ_{HCH}
S	HF/6-31G*	1.52736	1.08559	111.21533	107.67221
	HF/6-311+G**	1.52701	1.08631	111.19880	107.68976
	B3LYP/6-31G*	1.53066	1.09626	111.35280	107.52588
	B3LYP/6-311+G**	1.53089	1.09384	111.35547	107.52303
	MP2/6-311+G**	1.52925	1.09349	111.14651	107.74523
E	HF/6-31G*	1.54111	1.08460	111.65293	107.20411
	HF/6-311+G**	1.54104	1.08524	111.63206	107.22662
	B3LYP/6-31G*	1.54493	1.09515	111.78699	107.05943
	B3LYP/6-311+G**	1.54463	1.09271	111.77888	107.06822
	MP2/6-311+G**	1.54240	1.09264	111.62415	107.23510
Δ_{E-S}	HF/6-31G*	0.01375	-0.00099	0.43760	-0.46810
	HF/6-311+G**	0.01403	-0.00107	0.43326	-0.46314
	B3LYP/6-31G*	0.01427	-0.00111	0.43419	-0.46645
	B3LYP/6-311+G**	0.01374	-0.00113	0.42341	-0.45481
	MP2/6-311+G**	0.01315	-0.00085	0.47764	-0.51013

Table S2. LMOEDA results for rigid rotation of staggered conformer (B3LYP/6-311+G**).[a] Values are in kcal/mol.

Torsional angle (°)	ΔE_{es}	ΔE_{ex+rep}	ΔE_{pol}	ΔE_{disp}	ΔE_{int}	ΔE_{prep}	ΔE
0	-135.65	213.46	-160.93	-23.89	-107.01	18.49	-88.52
10	-135.64	213.28	-160.97	-23.89	-107.20	18.49	-88.71
20	-135.60	212.81	-161.07	-23.87	-107.72	18.49	-89.23
30	-135.55	212.15	-161.20	-23.84	-108.43	18.49	-89.94
40	-135.49	211.50	-161.34	-23.81	-109.14	18.49	-90.65
50	-135.46	211.02	-161.43	-23.79	-109.66	18.49	-91.17
60	-135.45	210.84	-161.47	-23.79	-109.85	18.49	-91.36

[a] ΔE_{es} = electrostatic energy, ΔE_{ex} = exchange repulsion energy, ΔE_{pol} = polarization energy, ΔE_{disp} = dispersion energy, ΔE_{int} = interaction energy, ΔE_{prep} = preparation energy, ΔE = total bonding energy.

Table S3. LMOEDA results for rigid rotation of eclipsed conformation (B3LYP/6-311+G**).[a] Values are in kcal/mol.

Torsional angle (°)	ΔE_{es}	ΔE_{ex+rep}	ΔE_{pol}	ΔE_{disp}	ΔE_{int}	ΔE_{prep}	ΔE
0	-130.74	203.08	-156.86	-23.66	-108.19	19.53	-88.66
10	-130.73	202.92	-156.89	-23.65	-108.36	19.53	-88.83
20	-130.70	202.49	-156.99	-23.63	-108.83	19.53	-89.30
30	-130.65	201.89	-157.11	-23.61	-109.48	19.53	-89.95
40	-130.61	201.30	-157.24	-23.58	-110.13	19.53	-90.60
50	-130.58	200.85	-157.33	-23.57	-110.61	19.53	-91.08
60	-130.56	200.69	-157.36	-23.56	-110.79	19.53	-91.26

[a] Labeling is the same as in Table S2.

Table S4. LMOEDA results for relaxed rotation of staggered conformer (B3LYP/6-311+G**).[a] Values are in kcal/mol.

Torsional angle (°)	ΔE_{es}	ΔE_{ex+rep}	ΔE_{pol}	ΔE_{disp}	ΔE_{int}	ΔE_{prep}	ΔE
0	-130.74	203.08	-156.86	-23.66	-108.19	19.53	-88.66
10	-130.93	203.27	-157.06	-23.67	-108.39	19.57	-88.82
20	-131.71	204.52	-157.83	-23.69	-108.70	19.39	-89.31
30	-132.87	206.46	-158.96	-23.72	-109.10	19.12	-89.98
40	-134.12	208.55	-160.17	-23.75	-109.48	18.82	-90.66
50	-135.11	210.26	-161.13	-23.78	-109.76	18.58	-91.18
60	-135.45	210.84	-161.47	-23.79	-109.85	18.49	-91.36

[a] Labeling is the same as in Table S2.